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Multi-GPU FFT Performance on Different Hardware Configurations

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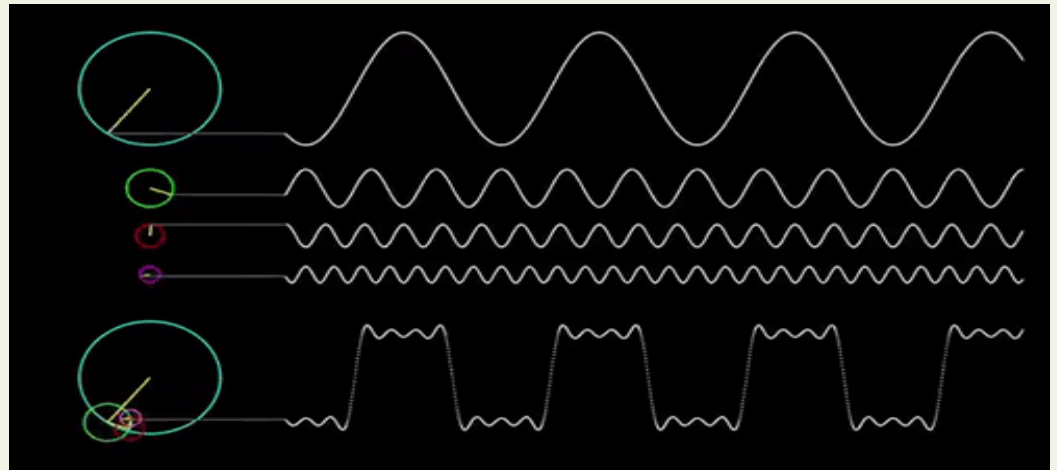


Advance Modeling & Simulation (AMS) Seminar Series
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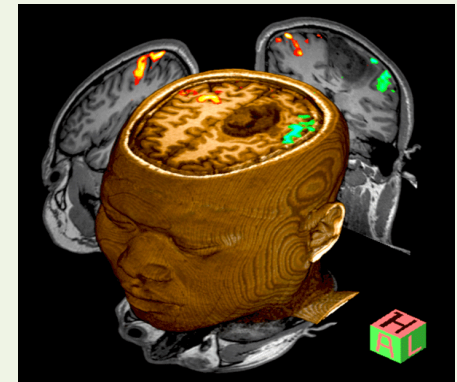
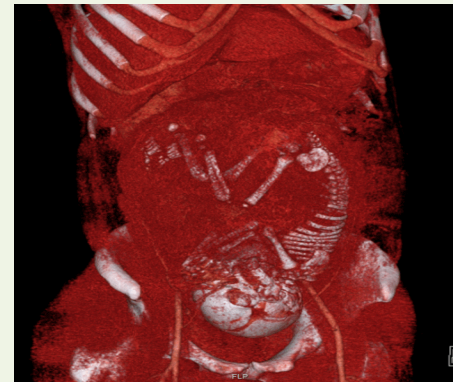
Fast Fourier Transform (FFT)

- **The Fourier transform**
 - Decomposes a function of time into the frequencies that make it up
 - Discretize then compute using FFTs
- **Motivating FFT based applications**
 - Digital Signal Processing (DSP)
 - Medical Imaging
 - Image Recovery
 - Computational Fluid Dynamics
 - Can require large datasets
- **Focus on large FFT problems that can not be solved in batch mode**
 - Benchmarking multi-GPU FFTs within a single node
 - CUDA functions
 - Collective communications
 - **Bandwidth and latency** will be strong factors in determining performance



Medical Imaging

- **Correct high resolution imaging can prevent a misdiagnosis**
- **Ultrasonic Imaging**
 - Creates an image by firing & receiving ultrasonic pulses into an object
 - Preferred technique for real-time imaging and quantification of blood flow
 - Provides excellent temporal and spatial resolution
 - Relatively inexpensive, safe, and applied at patient's bedside
 - Low frame rate
 - Traditional techniques do not use FFT for image formation
 - Pulse plane-wave imaging (PPI)
 - Utilizes FFTs for image formation
 - Improved sensitivity and can achieve much higher frame rates
- **Computed Tomography (CT)**
 - Removes interfering objects from view using Fourier reconstruction
- **Magnetic Resonance Imaging (MRI)**
 - Based on the principles of CT
 - Creates images from proton density, Hydrogen (^1H)
 - Image reconstruction by an iterative non-linear inverse technique (NLINV)
 - Relies heavily on FFTs
 - Real-time MRIs require fast image reconstruction and hence powerful computational resources



Medical Imaging (continued)

- **Multi-Dimensional requirements**

- 2D, 3D, and 4D imaging
- Traditional CT & MRI scans produce 2D images
- Static 3D Volume (brain, various organs, etc.)
 - Combining multiple 2D scans
- Moving objects incorporate time
 - 3D video image: multiple 2D images over time
 - 4D video volume: multiple 3D volumes over time

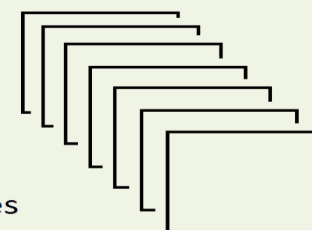
- **Supplementary techniques also require FFTs**

- Filtering operations
- Image reconstruction
- Image analysis
 - Convolution
 - Deconvolution

2D
One image of size
512 x 512



3D
One volume of size
512 x 512 x 512



4D
Many volumes
128 x 128 x 64 x 1000

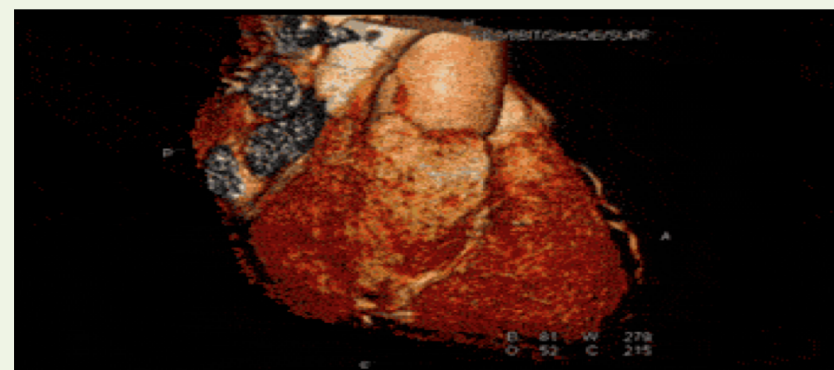
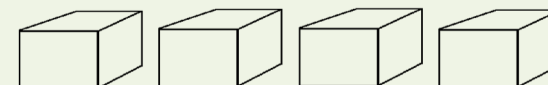
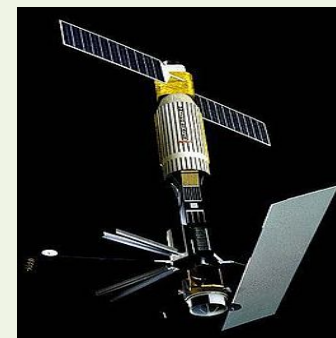


Image Recovery

- Ground based telescopes require enhanced imaging techniques to compensate for atmospheric turbulence
 - Adaptive Optics (AO) can reduce the effect of incoming wavefront distortions by deforming a mirror in order to compensate in real time
 - AO cannot completely remove the effects of atmospheric turbulence
 - Multi-frame Blind Deconvolution (MFBD) is a family of “speckle imaging” techniques for removing atmospheric blur from an ensemble of images
 - Linear forward model: $\mathbf{d}_m(\mathbf{x}) = \mathbf{o}(\mathbf{x}) * \mathbf{p}_m(\mathbf{x}) + \sigma_m(\mathbf{x})$
 - Each of m observed data frames of the image data ($\mathbf{d}_m(\mathbf{x})$) is represented as a pristine image ($\mathbf{o}(\mathbf{x})$) convolved with a Point Spread Function ($\mathbf{p}_m(\mathbf{x})$) as well as an additive noise term ($\sigma_m(\mathbf{x})$) that varies per image.
 - Ill-posed inverse problem solved with max likelihood techniques and is very computationally intense
 - Requires FFTs in its iterative process to calculate the object, producing a “crisper” image

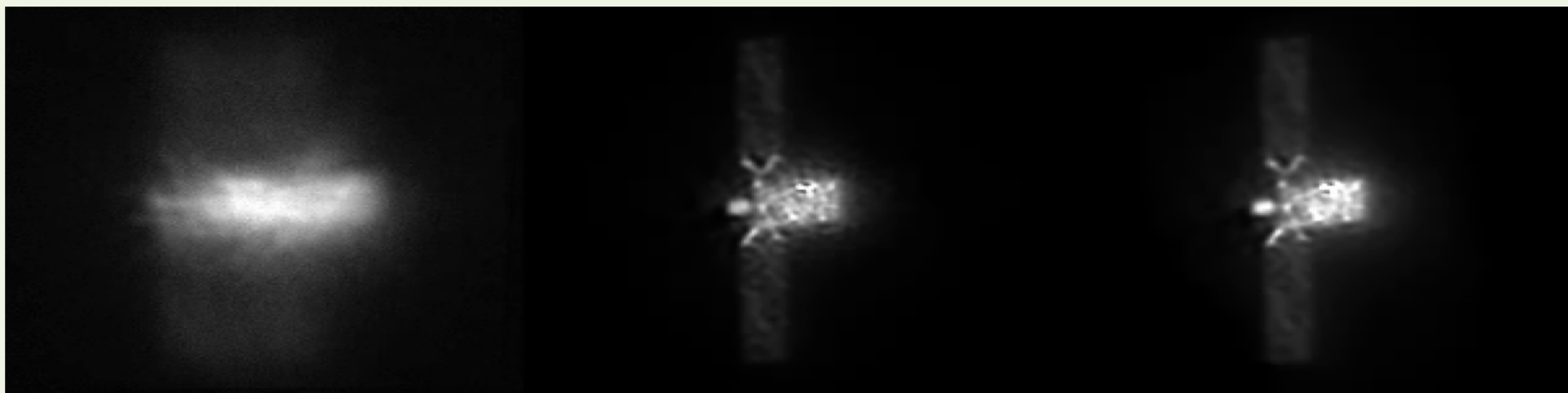


Seasat



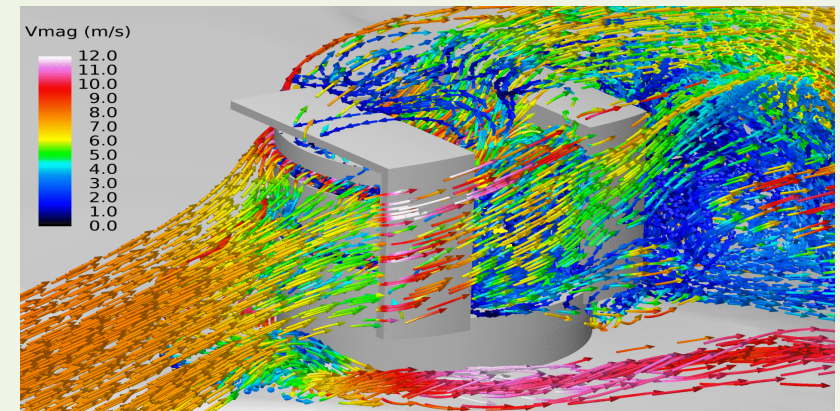
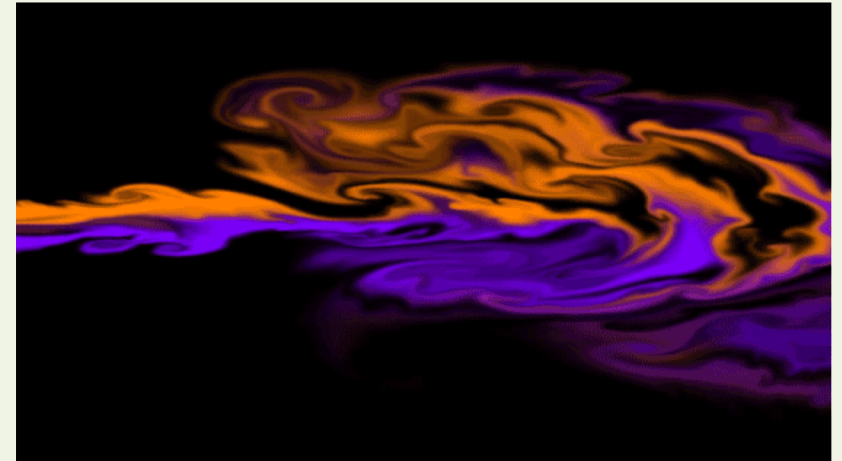
Image Recovery (continued)

- **Physically Constrained Image Deconvolution (PCID)**
 - A highly effective MFBD has been parallelized to produce restorations quickly
 - A GPU version of the code is in development
- **Fermi Gamma-ray Space Telescope: NASA satellite (2008)**
 - Study astrophysical and cosmological phenomena
 - Galactic, pulsar, other high-energy sources, and dark matter



Computational Fluid Dynamics

- **Direct Numerical Simulation (DNS)**
 - Finite Difference, Finite Element, & Finite Volume methods
 - **Pseudo Spectral method**: effectively solving in spectral space using FFTs
- **Simulating high resolution turbulence**
 - Requires large computational resources
 - Large % of time spent on forward and inverse Fourier transforms
 - Effective performance can be small due to its extensive communication costs
 - Performance would be improved with higher bandwidth and lower latency
- **Code examples that utilize FFTs on GPUs**
 - NASA's FUN3D
 - Tarang
 - UltraFluidX



Benchmarking Multi-GPU FFTs

- **Represent large 3D FFTs problems that cannot fit on a single GPU**
 - Single precision Complex to Complex (C2C) in-place transformations
 - C2C considered more performant than the Real to Complex (R2C) transform
 - In-place – reduces memory footprint and requires less bandwidth
- **Distributing large FFTs across multiple GPU**
 - Communication is required when spreading and returning data
 - Significant amount collective communications
 - Bandwidth and latency will be strong factors in determining performance
- **Primary CUDA functions (used v9.1 for consistency across platforms)**
 - *cufftXtSetGPUs* – identifies the GPUs to be used with the plan
 - *cufftMakePlanMany64* - Create a plan that also considers the number of GPUs available. The “64” means argument sizes and strides to be 64 bit integers to allow for very large transforms
 - *cufftXtExecDescriptorC2C* – executes C2C transforms for single precision

Hardware Configurations Examined

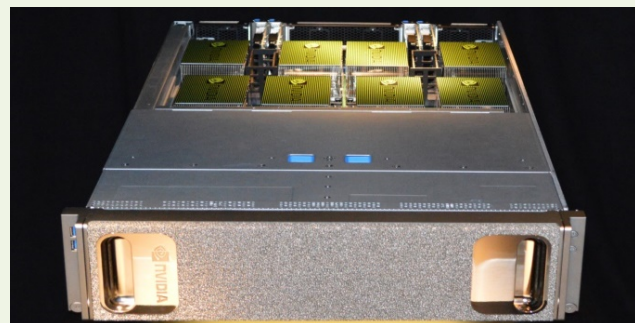


- **IBM Power 8**
 - Hokulea (MHPCC)
 - Ray (LLNL)
- **IBM Power 9**
 - Sierra (LLNL)
 - Summit (ORNL)



NVIDIA

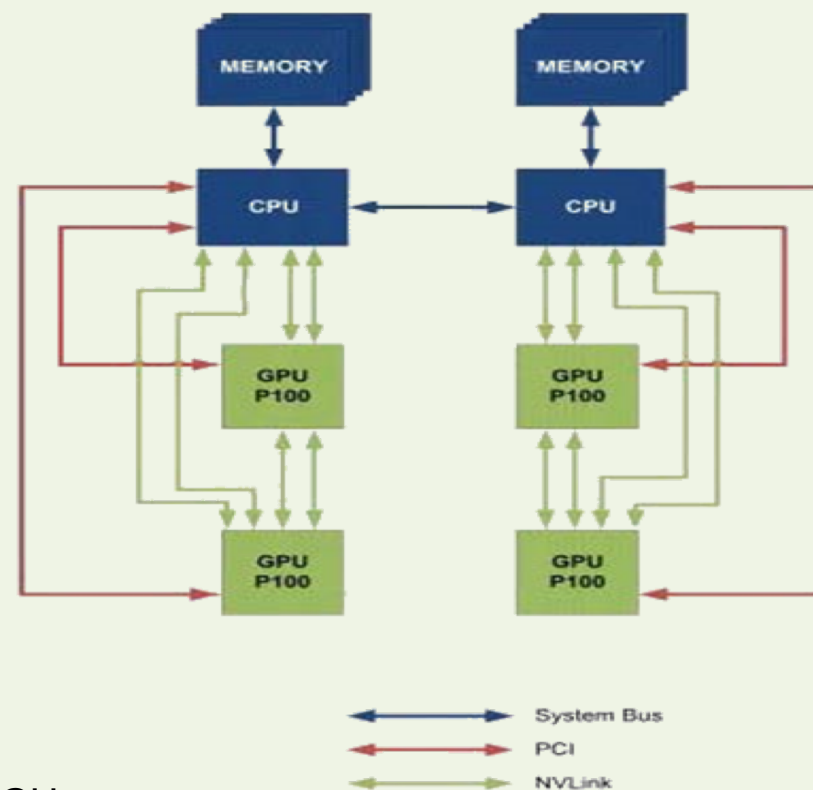
- **x86 PCIe**
- **Nvidia DGX-1 (Volta)**
- **Nvidia DGX-2**
- **Nvidia DGX-2H**



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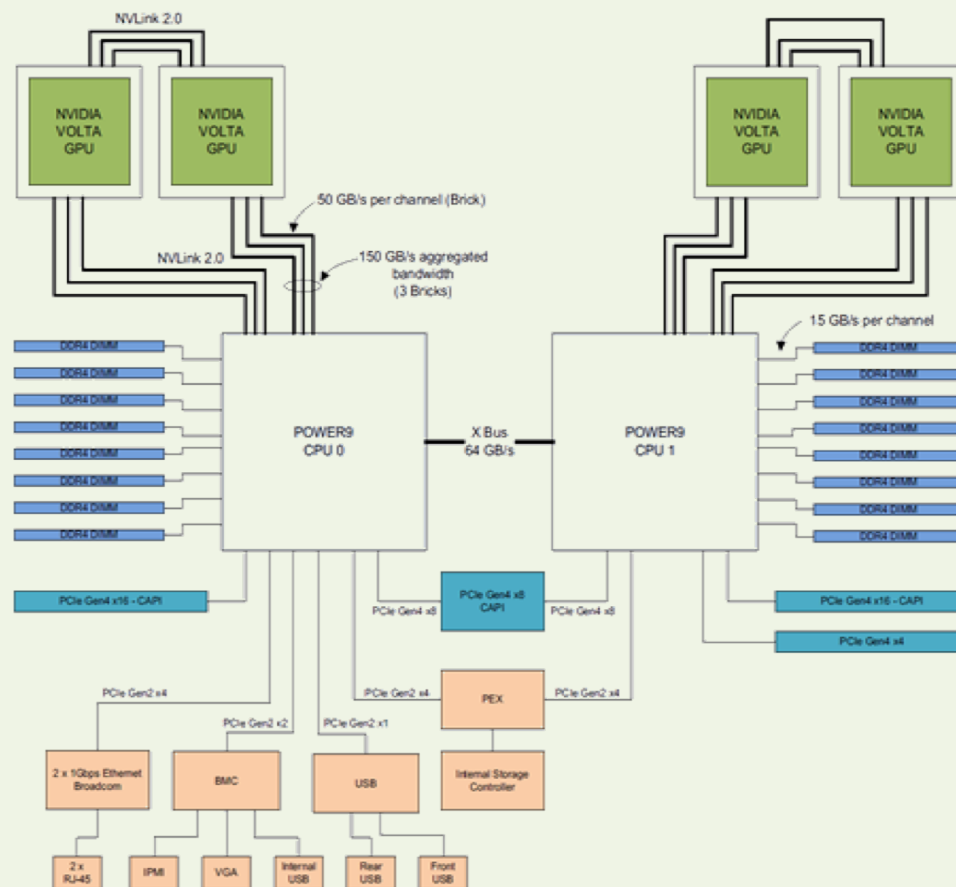
IBM POWER8 with P100 (Pascal) GPUs

- 2x P8 10 core processors
- 4x NVIDIA P100 GPUs
 - NVIDIA NVLink 1.0
 - 20 GB/s unidirectional
 - 40 GB/s bidirectional
 - 4 NVLink 1.0 lanes/GPU
 - 2 lanes between neighboring GPU
 - 2 lanes between neighboring CPU
- X-Bus between CPUs
 - 38.4 GB/s
- POWER AI switch can be enabled
 - Increases P100 clock speed from 1328 GHz to 1480 GHz



IBM POWER9 with Volta GPUs

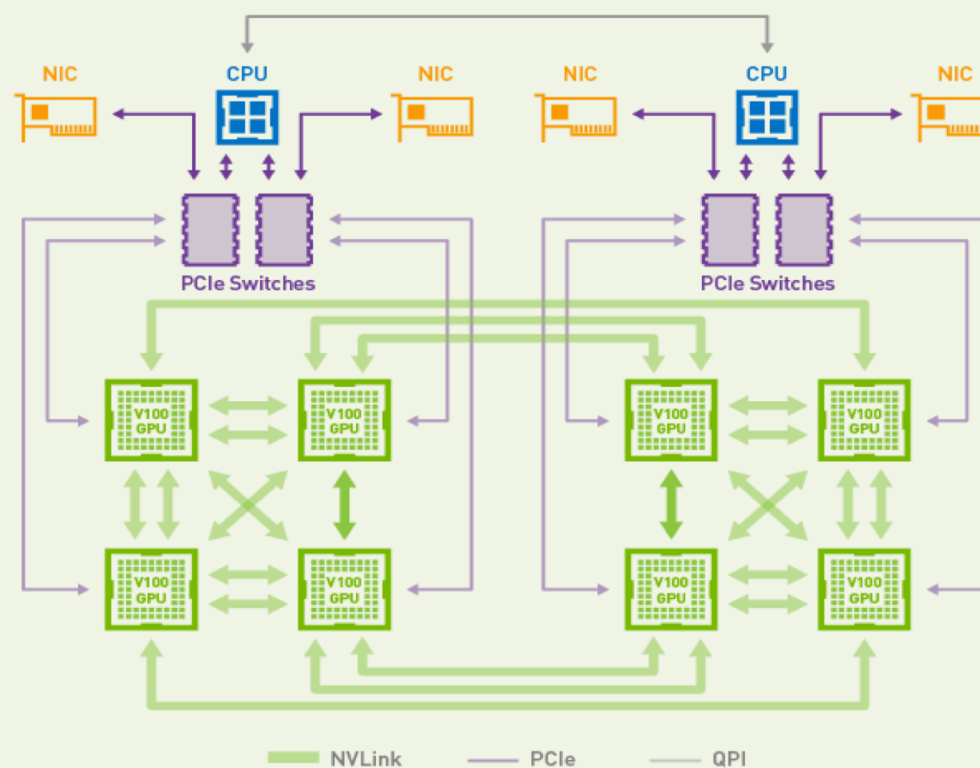
- **2x P9 22 core processors**
- **4x or 6x NVIDIA V100 GPUs**
 - NVIDIA NVLink 2.0
 - 25 GB/s unidirectional
 - 50 GB/s bidirectional
 - 6 NVLink 2.0 lanes/GPU
- **4x GPUs/node**
 - 3 lanes between neighboring GPU
 - 3 lanes between neighboring CPU
- **6x GPUs/node**
 - 2 lanes between neighboring GPU
 - 2 lanes between neighboring CPU
- **X-Bus between CPUs**
 - 64 GB/s



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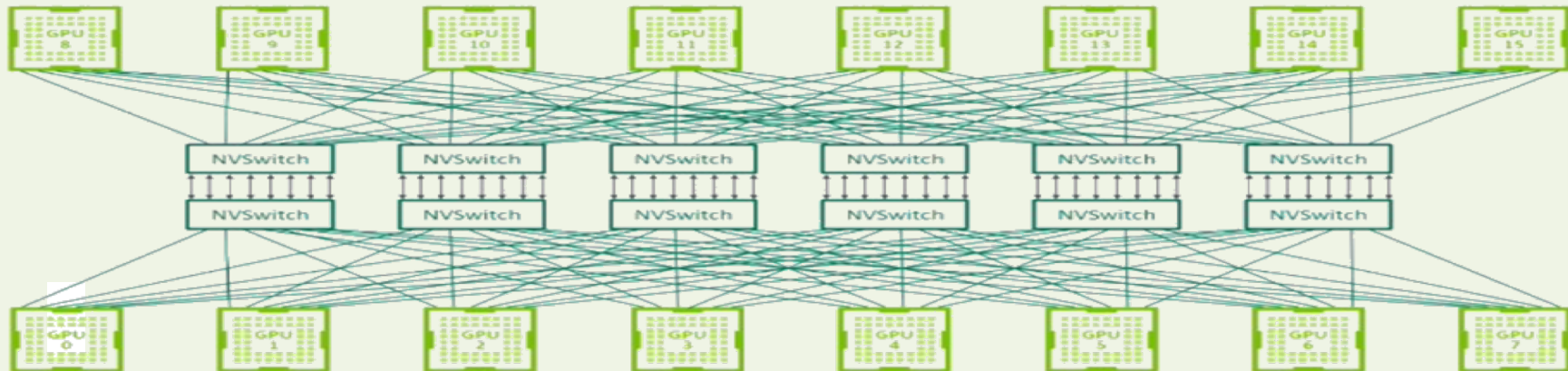
DGX-1v with 8 V100 GPUs

- 2x Intel Xeon E5-2698 v4, 20-core
- 8x NVIDIA V100 GPUs
 - NVIDIA NVLink 2.0
 - 25 GB/s unidirectional
 - 50 GB/s bidirectional
- Hybrid cube mesh topology
 - Variable lanes/hops between GPUs
 - 2 lanes between 2 neighboring GPUs
 - 1 lane between 1 GPU neighbor
 - 1 lane per cross CPU GPU
 - 2 hops to other cross CPU GPUs
 - PCIe Gen3 x16
 - 32 GB/s bidirectional
 - GPU & PCIe switch
 - PCIe switch & CPU



DGX-2 with 16 V-100s

- 2 Dual Intel Xeon Platinum 8168, 2.7 GHz, 24-cores
- 16x NVIDIA 32GB V100 GPUs
- NVSwitch/NVLink 2.0 interconnection
 - Capable of 2.4 TB/s of bandwidth between all GPUs
 - Full interconnectivity between all 16 GPUs



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3D FFT (C2C) Performance Study

- **IBM Power Series**

- IBM P8 (4x 16GB P100s) & IBM P9 (4x 16GB V100s)
- Multiple sized cases from 64x64x64 to 1280x1280x1280 (memory limited)
- 4 cases that shows how bandwidth & latency can affect performance:
 - 1 GPU only connect to CPU with NVLink
 - 2 GPUs attached to the same CPU and connected with NVLink
 - 2 GPUs attached to different CPUs
 - 4 GPUs (2 attached to each CPU)



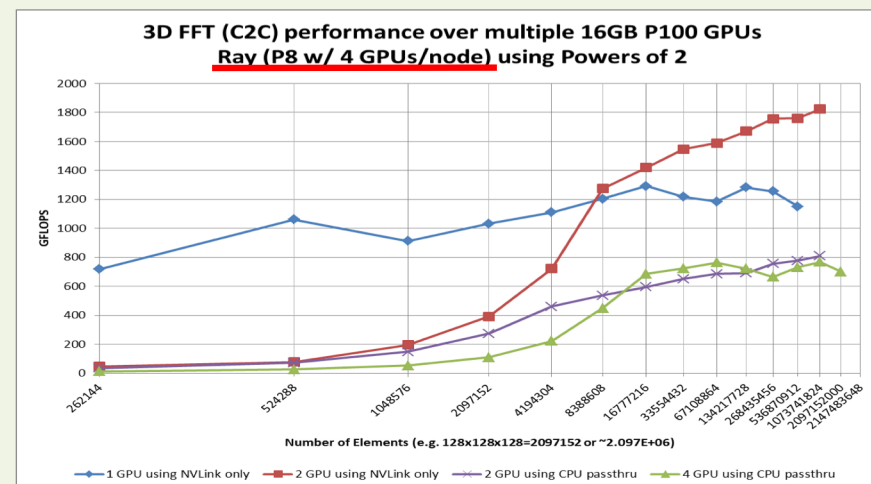
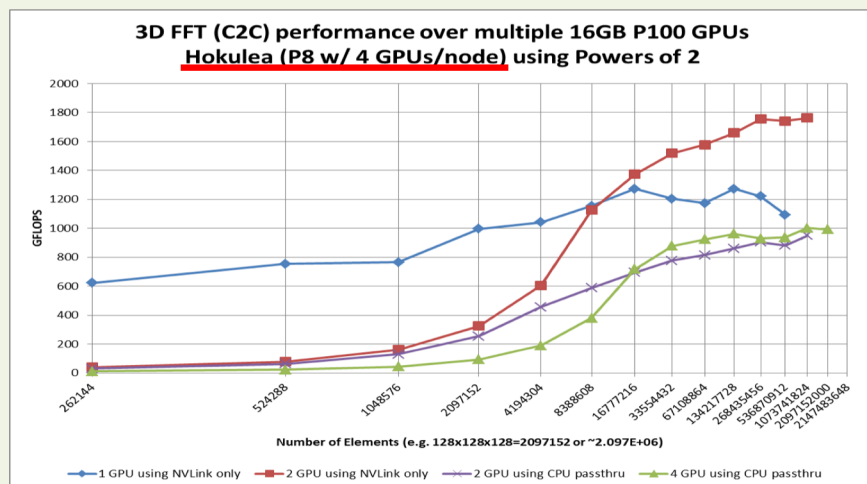
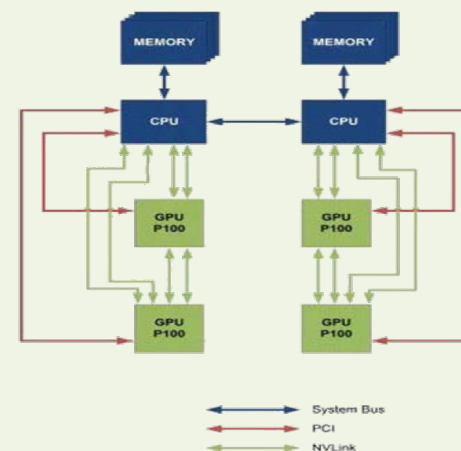
- **x86 based systems**

- Multiple sized cases from 64x64x64 to 2048x2048x2048 (memory limited)
- PCIe connected GPU (no NVLink) system (PCIe G3 16x – 16GB/s bandwidth)
 - 1, 2, & 4 GPU cases
- DGX-1v
 - 1, 2, 4, & 8 GPU cases
- DGX-2
 - 1, 2, 4, 8, & 16 GPU cases



IBM P8 Performance Study

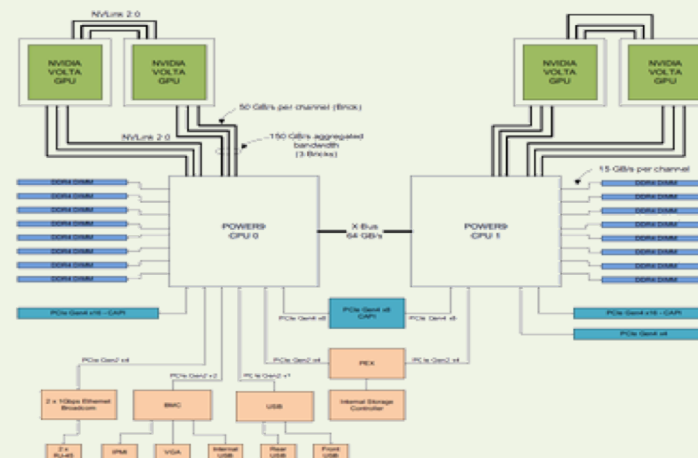
- **Very similar performance between the 2 IBM P8s**
 - Only noticeable difference is the CPU pass-through cases
 - Better performance for non-CPU pass-through cases
 - Power AI: negligible effect as the limiting factor was bandwidth and latency
- **Same-socket 2x GPU case**
 - Bandwidth/latency has not dramatically affected performance before the problem size has reached its memory limit
- **All other GPU cases are more affected by bandwidth & latency**



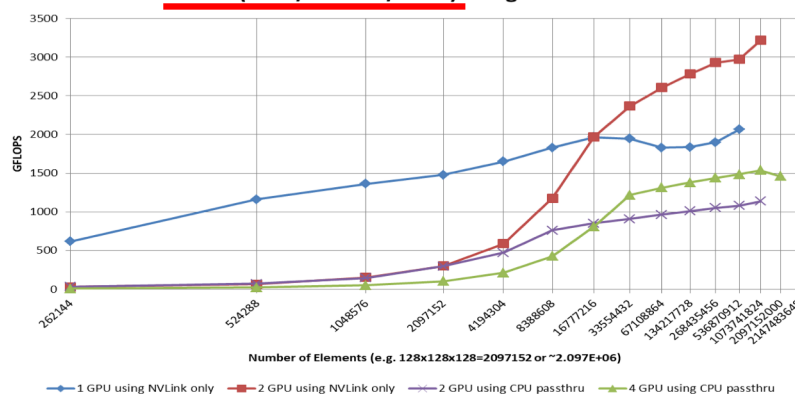
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IBM P9 Performance Study

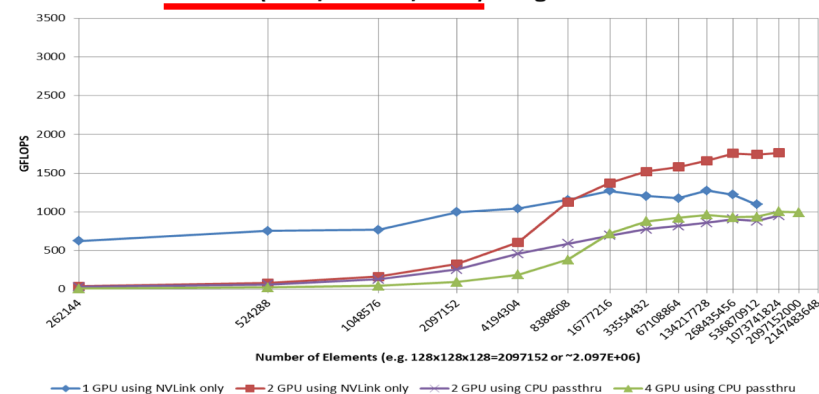
- **P9 with 4x 16GB V100s performed better than the P8**
 - Similar trends in performance as P8 b/c of architecture
 - Better overall performance b/c of V100 and 6 NVLink 2.0 lanes
 - Additional bandwidth of NVLink 2.0 allowed for better scaling
- **2x & 4x GPU CPU pass-through cases**
 - Bandwidth & latency limit performance gain
- **Summit performance expectation w/ 6 GPUs/node**
 - Less available lanes per GPU \equiv less bandwidth
 - Greater Memory (6x16GB) \equiv greater number of elements



**3D FFT (C2C) performance over multiple 16GB V100 GPUs
Sierra (P9 w/ 4 GPUs/node) using Powers of 2**



**3D FFT (C2C) performance over multiple 16GB P100 GPUs
Hokulea (P8 w/ 4 GPUs/node) using Powers of 2**



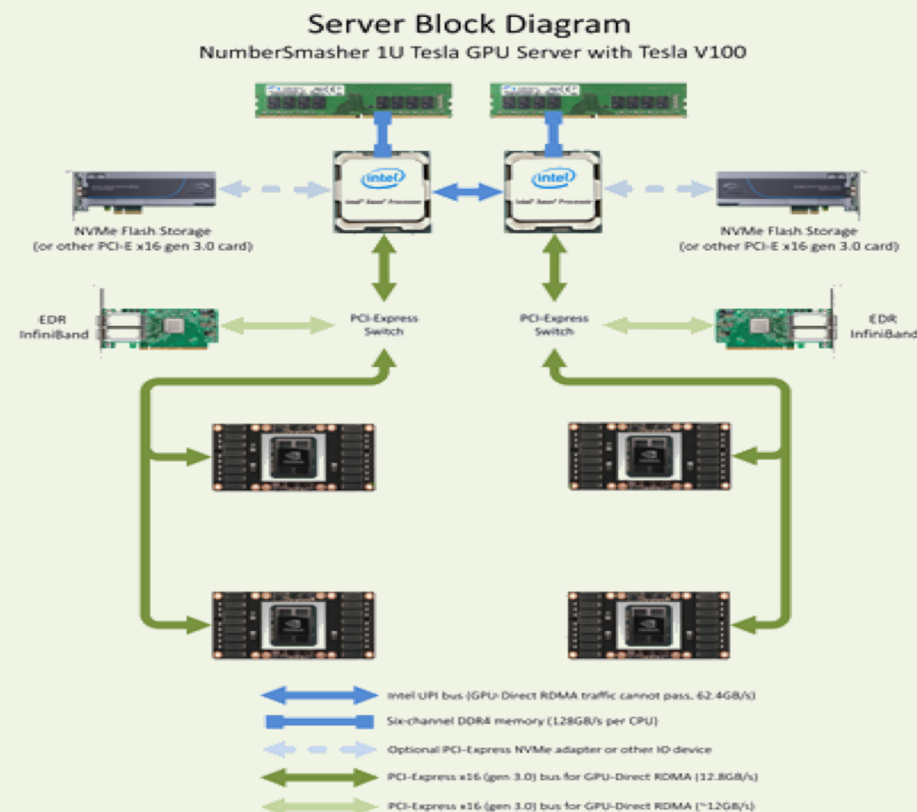
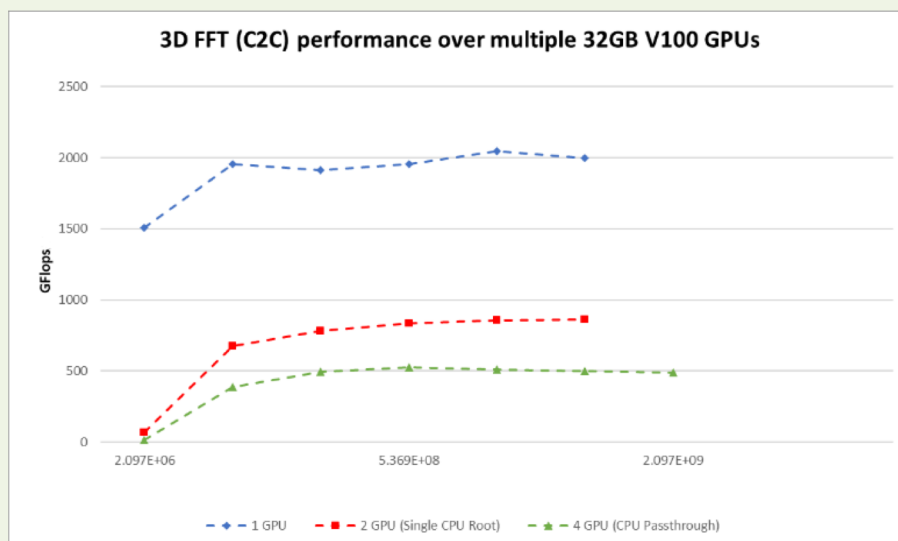
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x86 PCIe Based Performance Study

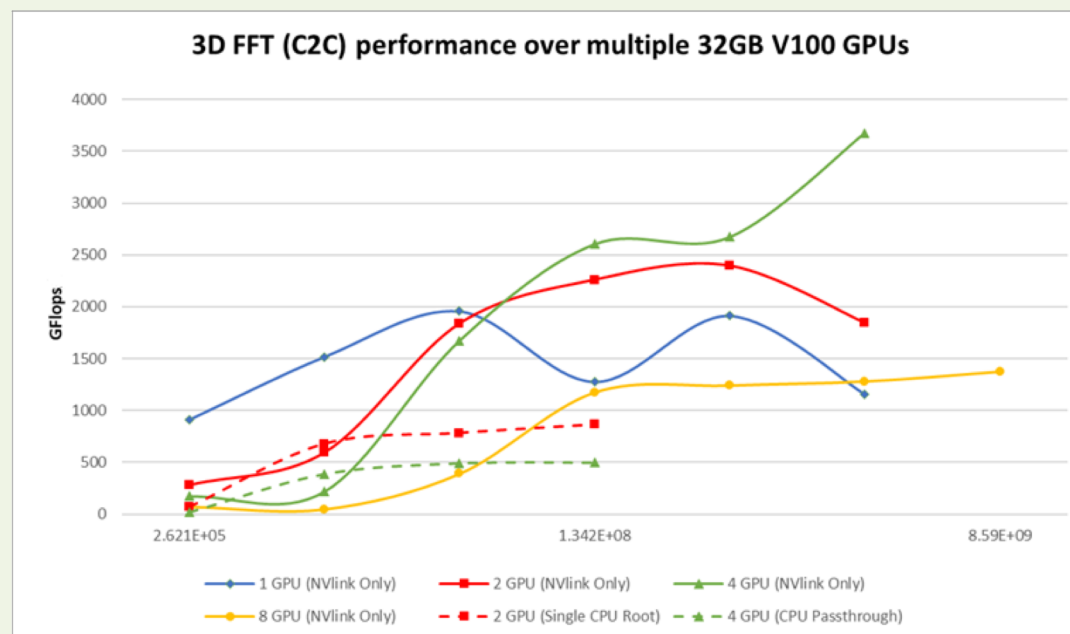
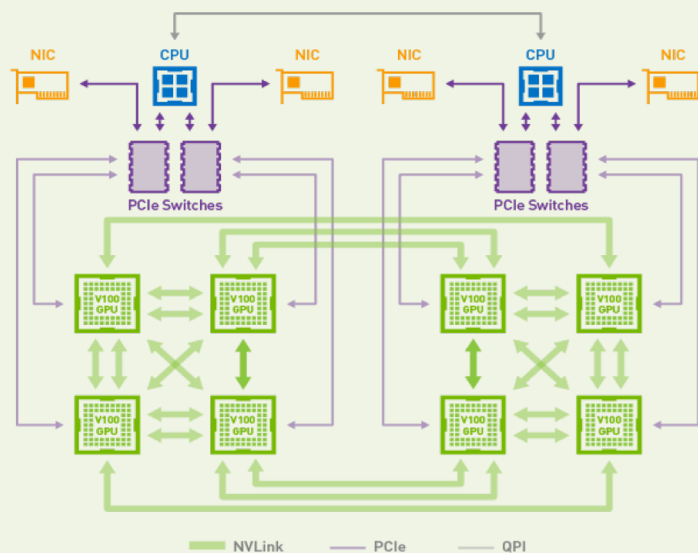
- 4x V100 (32GB) GPUs connected via x16 G3 PCIe (no NVLink)
 - Communication saturates the PCIe bus resulting in performance loss
 - Also limited by the QPI/UPI communication bus
 - The 3D FFT does not scale



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DGX-1v Performance Study

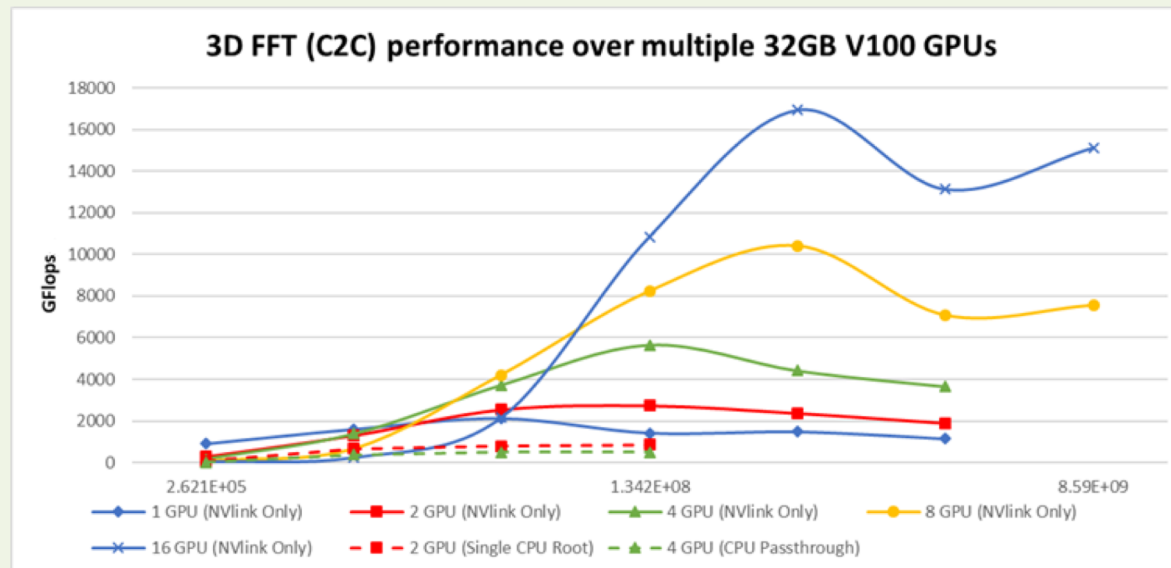
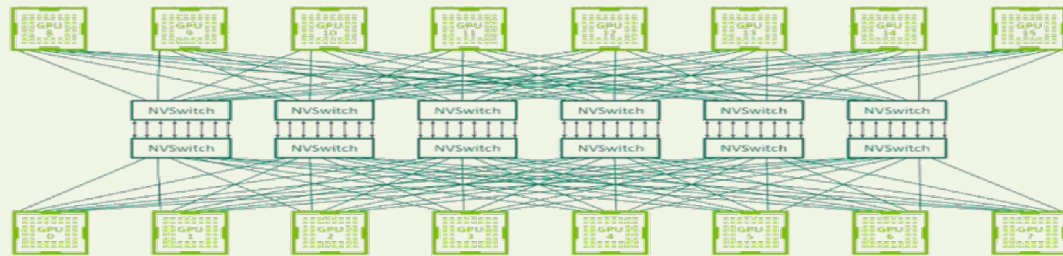
- **8x 32GB V100 GPUs**
 - 4 GPUs/CPU socket
- **Hybrid Mesh Cube topology**
 - Mix of NVLink connectivity
- **Variety of comm. cases**
 - NVLink 2.0
 - PCIe on same socket
 - PCIe with CPU pass-through



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DGX-2 Performance Study

- 16x 32GB V100 GPUs
 - NVSwitch/NVLink
- Variety of comm. cases
 - NVLink 2.0
 - PCIe on same socket
 - PCIe with CPU pass-through

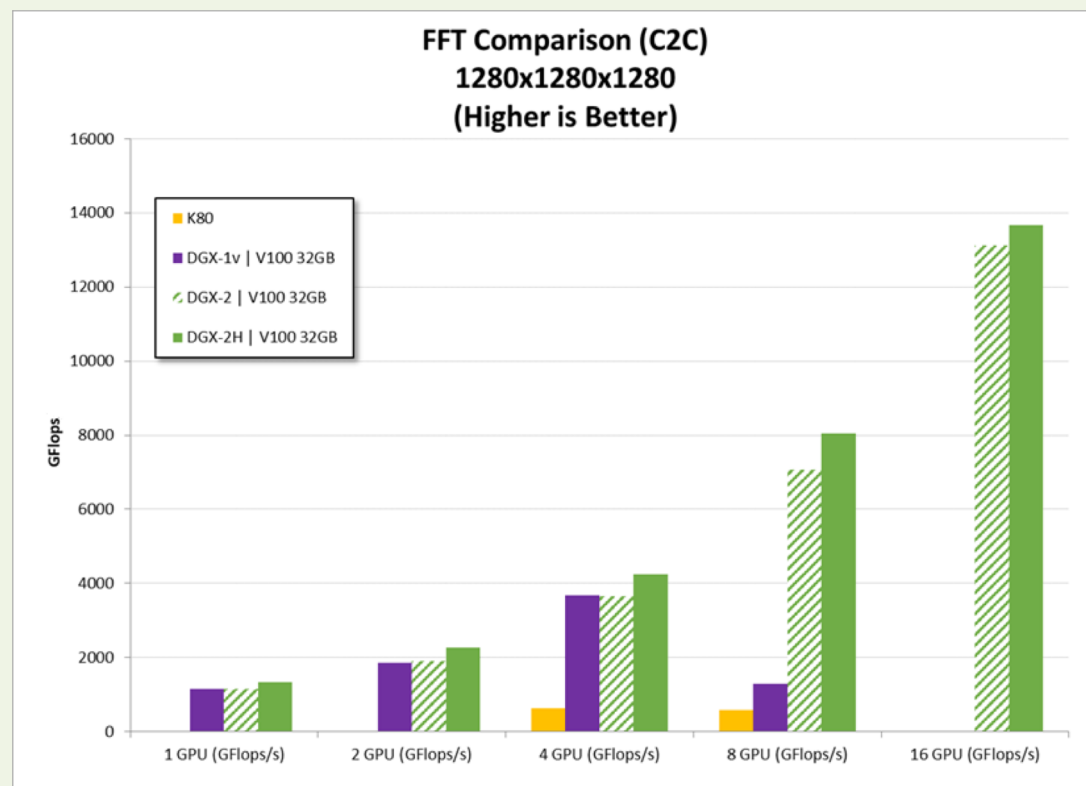
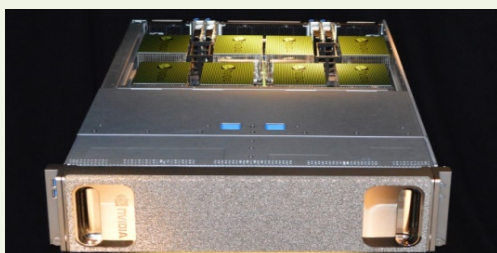


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DGX-1v, DGX-2, DGX-2H Comparison

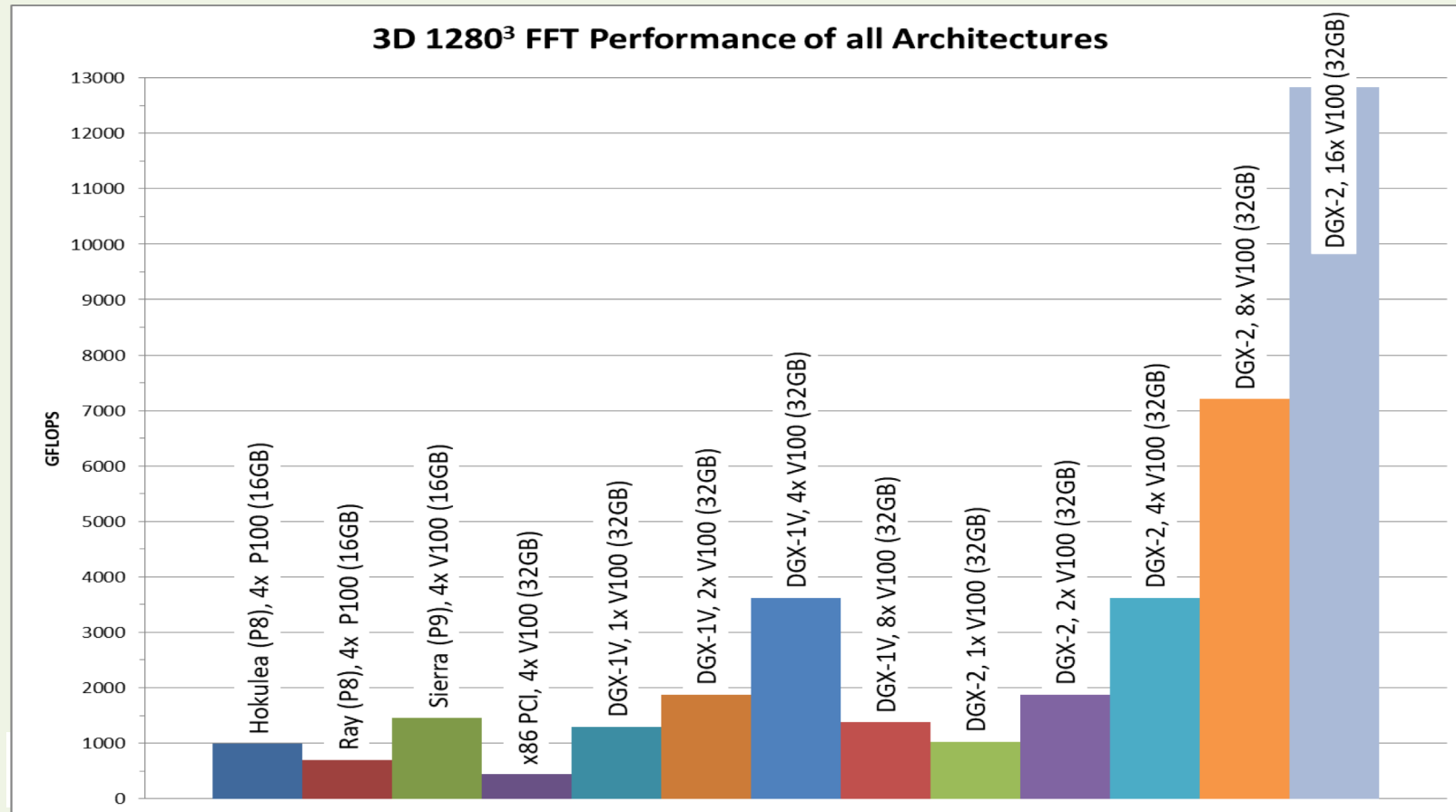
- **Key takeaways**

- Very similar performance up to 4 GPUs
- DGX-1v overhead for 8 GPU in the Hybrid Mesh Cube topology
- DGX-2H performs ~10-15% better than the DGX-2



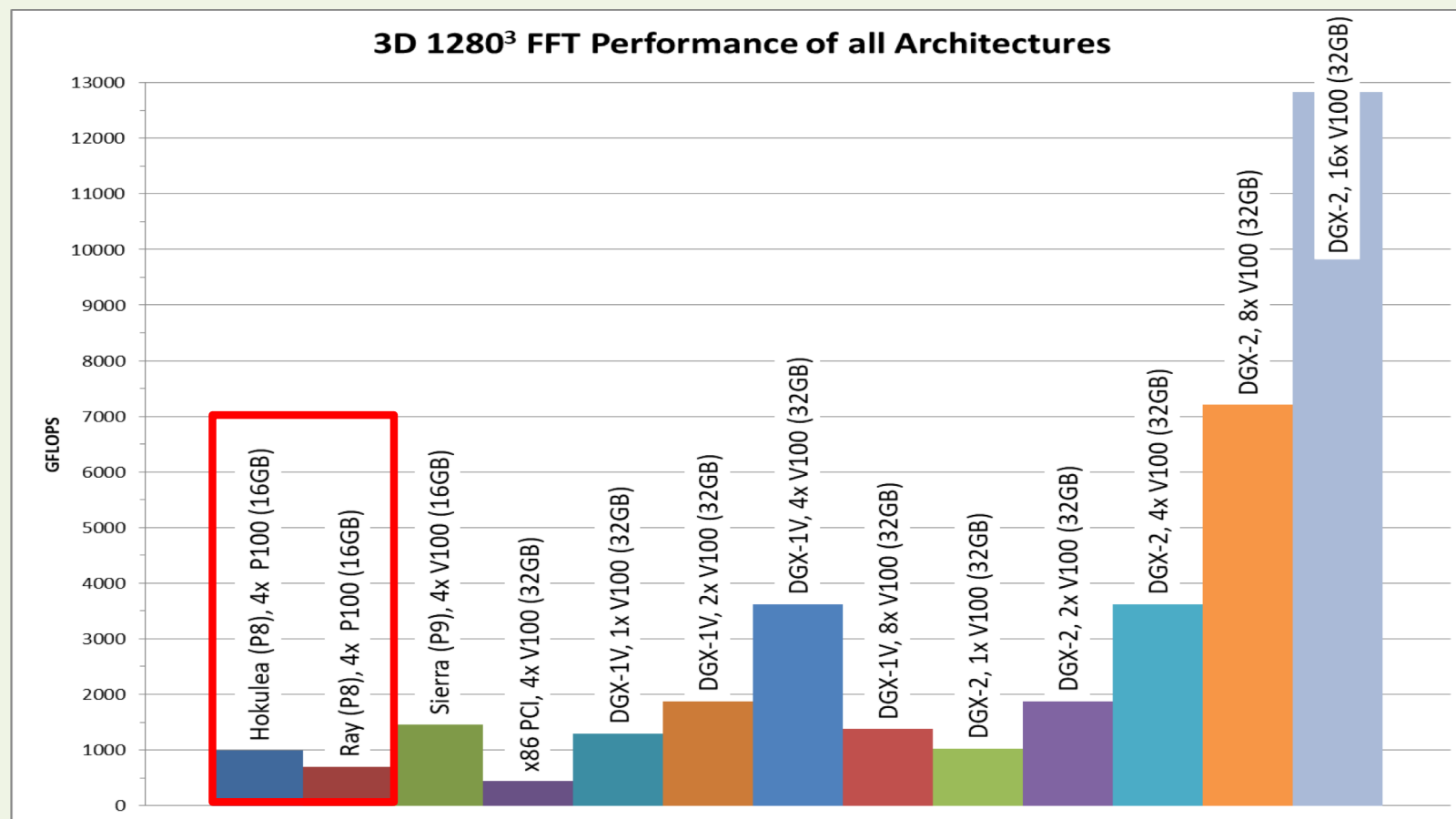
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Collective Performance



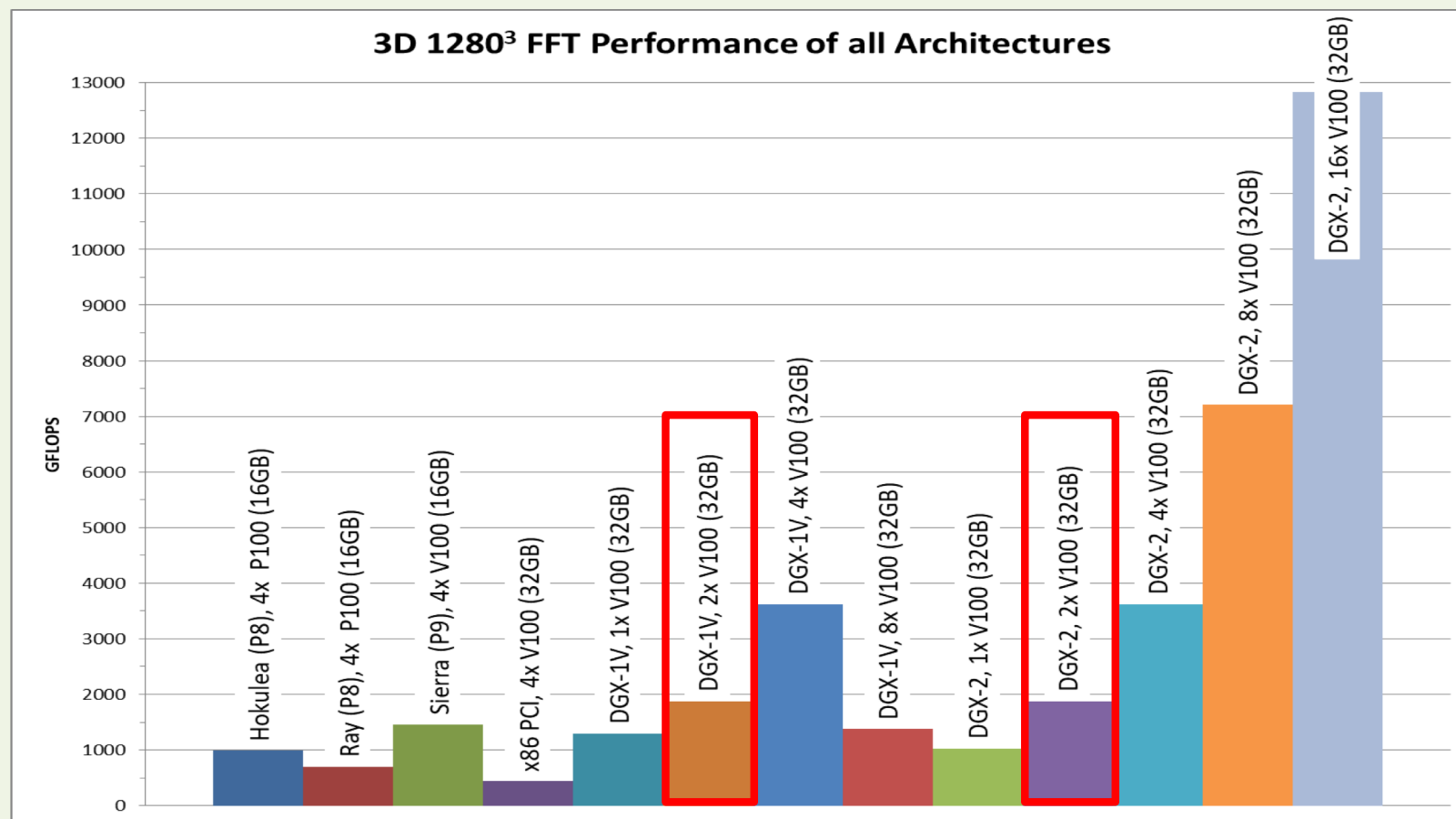
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4x P100s (16GB) Performance



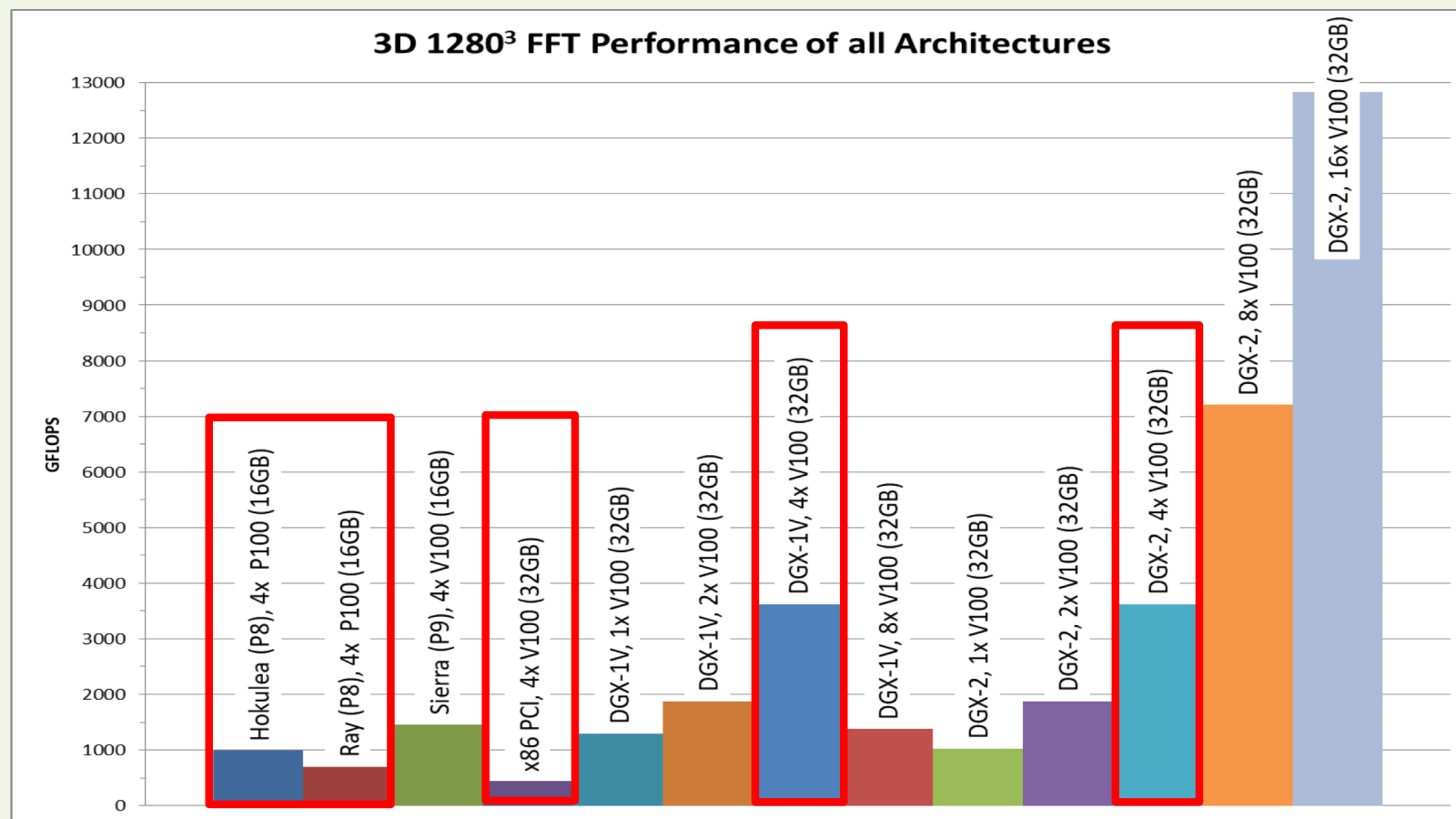
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2x V100 (32GB) Performance



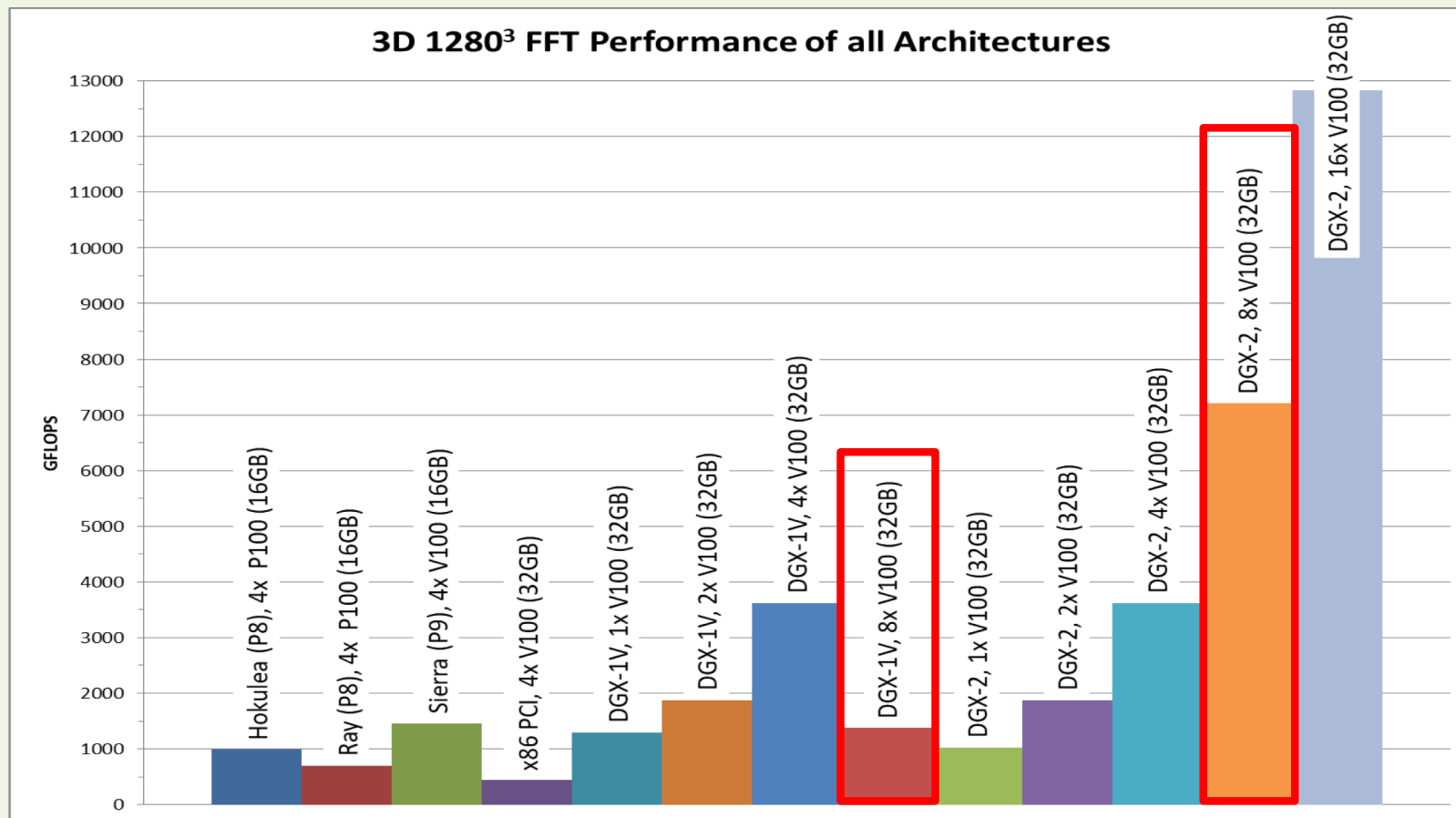
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4x V100 Performance



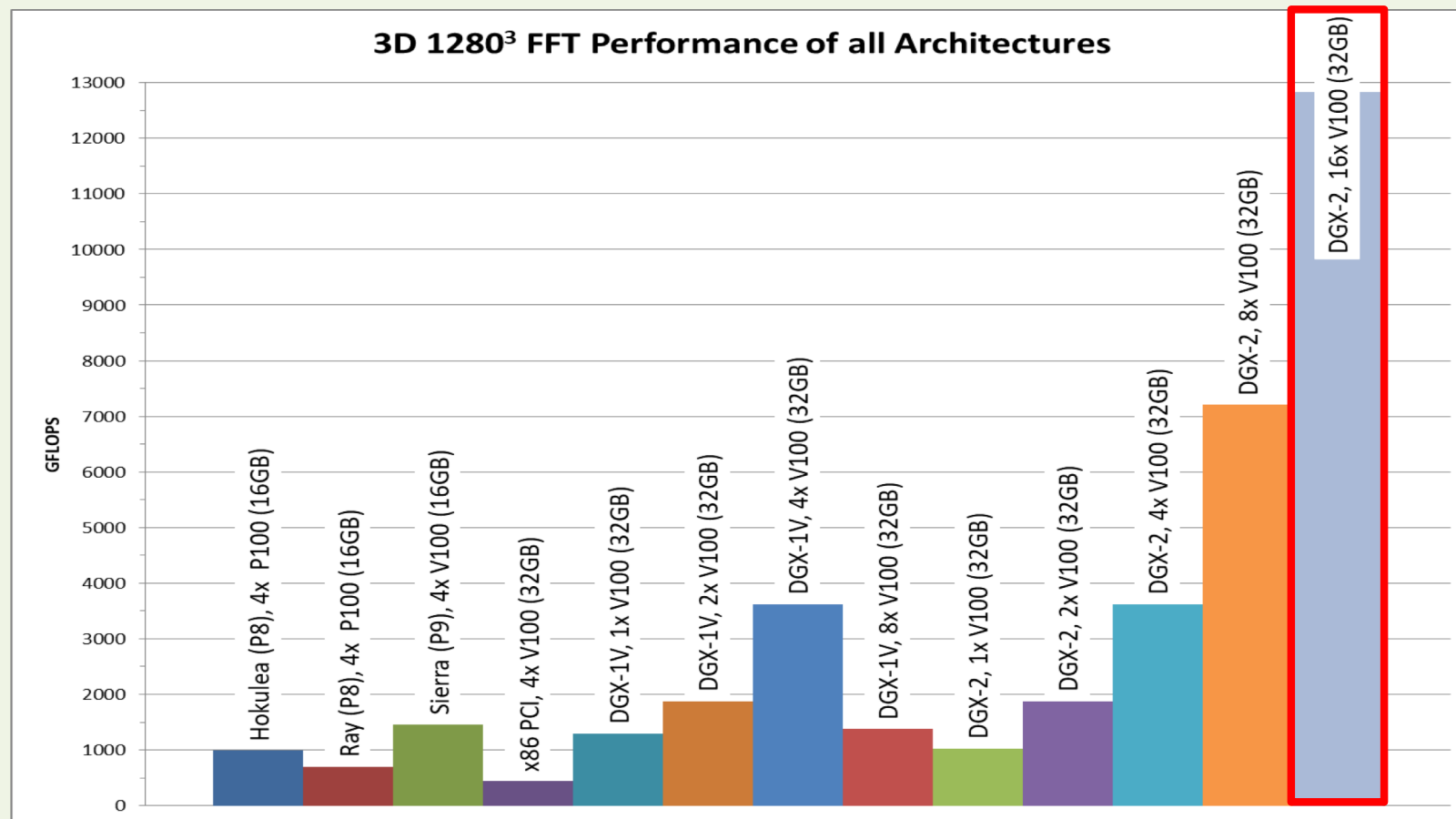
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8x V100 (32GB) Performance




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16x V100 (32GB) Performance



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Conclusions

- 
- **Collective communication operations dominate performance when large FFTs are spread over multiple GPUs**
 - Highly dependent on underlying architecture's bandwidth and latency
 - **x86 PCIe based systems**
 - Lower bandwidth and higher latency restrict scaling of multi-GPU FFTs
 - **IBM Power Series**
 - Overhead associated when needed to handle communication between GPUs on different sockets limit performance
 - **NVIDIA DGX-1v**
 - Hybrid Mesh Cube topology lowers communication overhead between GPUs
 - **NVIDIA DGX-2**
 - NVSwitch technology has the lowest communication overhead between GPUs
 - **NVIDIA DGX-2H**
 - Low communication overhead combined with faster GPUs

Future Work

- **Future Work**

- Examine Unified Memory FFT implementations
- Multi-node Multi-GPU FFT implementations
- Deeper analysis of the DGX-2H

- **Acknowledge support by**

- The U.S. DoD High Performance Computing Modernization Program
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- NVIDIA